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Abstract

Being a three body problem, the scattering of an incoming antiproton (p^-) by a hydrogen atom (H, consisting of an electron, e^-, bound to a proton, p) is one of the simplest problems in quantum mechanics that requires a numerical solution. An appropriate choice of calculational method for this system depends on the energy of the p^-. Described and compared here are three methods, valid in essentially separate energy ranges from zero energy through MeV energies. In spite of its seeming simplicity, much effort is required in terms of mathematical manipulation and use of approximations to render this problem capable of numerical solution.

1. Introduction

The system consisting of three particles, a proton (p, with unit positive charge), an antiproton (p^-, unit negative charge), and an electron (e^-, unit negative charge) is one of the simplest systems for which exact, analytic solutions of their quantum mechanical motion are yet to be found. Hence the need for a numerical solution to the particular problem considered here, the scattering of an incident p^- by a stationary hydrogen atom (H, p-e^- bound in the ground state). Calculational methods for solving this problem vary considerably, depending in part on what physical processes are possible for the given incident energy of the p^- on the stationary H.

At all energies a possible outcome of the scattering is that the p^- is deflected with no permanent effect on the H (elastic scattering). At incident energies around and above about 40 eV, other processes are possible in which the hydrogen atom becomes excited or ionized (forms of inelastic scattering). In these processes the p^- transfers part of its energy to the e^-. At lower energies, these inelastic processes rapidly decrease and then cease (at specific energies) when the p^- energy is insufficient to cause direct ionization or a particular level of excitation. However, for energies around and below 27.2 eV, another process is possible in which the p^- is captured into a bound state with the p, forming protonium. The electron then departs since it cannot be bound to protonium, so this is another form of ionization. In this latter process the e^- can absorb very little energy beyond the minimum required for ionization. That energy is 13.6 eV, so when the inci-

dent p^- energy is increasing in the vicinity of 27.2 eV, which corresponds to 13.6 eV in the center-of-mass frame, the probability of protonium formation and the accompanying indirect ionization drops rapidly to zero.

The choice of calculational method also depends on properties of the solution that can be foreseen without obtaining a full, accurate solution. As explained later, this suggests, at all but the lowest energies, treatment of the p^- as a classical particle interacting with the quantum mechanical H. Hence the designation, semiclassical approximation, which can be shown to have at least a significant level of validity for all energies around and above about 10^{-4} eV. Concurrently, it may be shown for energies in this same range that the p^- portion of the solution involves many waves of quantized angular momentum. Thus in this range, fully quantum methods that involve expansions in basis sets of p^- wave functions lead to a prohibitively large number of coupled differential equations for current numerical capabilities.

Described here are the equations that must be solved and three particular methods of solution that span the energy range of the incident p^- form zero 1 MeV.

2. Equations to Solve

The ordinary Schroedinger equation determines the non-relativistic quantum mechanical motion of the three particles. It is (using atomic units in which the unit of mass is the mass of the electron, of distance one Bohr radius, of charge the proton charge, and of angular momentum Plank's constant over 2π)

$$-i\,\partial\Psi/\partial t = H\Psi \tag{1}$$

for the time dependent form and

$$H\psi = E\psi \tag{2}$$

for the time independent form, where t is the time, H the Hamiltonian operator, E the total energy of the particles, and Ψ and ψ are the wave functions to be solved for. Ψ and ψ are both functions of the spatial coordinates of the particles, and Ψ is additionally a function of time. H is given by

$$H = K + V\,, \tag{3}$$

where K is the kinetic energy operator and V is the potential energy. Here, after the center of mass motion has been separated out (and employing atomic units), K is given by

$$K = -(1/2\mu_e)\nabla_r^2 - (1/\mu_p)\nabla_R^2 - (1/\mu_p)\nabla_r\cdot\nabla_R\,, \tag{4}$$

where $\mu_e = m_p/(m_e+m_p)$ and $\mu_p = m_p/m_e$, with m_e being the mass of the e^- and m_p the common mass of the p and p^-. The ∇'s are gradient operators or, when squared, Laplacians. Their subscripts denote to which coordinate set they refer, with r denoting the

coordinates of the e^- relative to the p and R the coordinates of the p^- relative to the p. Here, V is given by

$$V = -1/r - 1/R + 1/\rho \,, \tag{5}$$

where r is the distance between the p and e^-, R is the distance between the p and p^-, and ρ is the distance between the e^- and p^-. Some other choices of coordinates lead to only the Laplacians appearing in K, but the choice shown here, which includes the gradient product, is more convenient for expressing initial and final conditions in Eq. (1) and boundary conditions in Eq. (2).

Eq. (1) determines Ψ uniquely at all times if its form is known for one particular time. Likewise Eq. (2) determines ψ uniquely for a given E and a given set of boundary conditions. Eq. (1) and Eq. (2) are closely related in that Eq. (1) may be easily solved by expanding Ψ in the form $\Psi = \Sigma_j \exp[-iE_jt]\psi_j$, where ψ_j are the eigenstates that result from solving Eq. (2) for all possible values of E and relevant boundary conditions. Whether one chooses to solve Eq. (1) or Eq. (2) for a particular p^--H scattering problem depends on the approximations and numerical methods chosen.

The approximations and numerical methods suitable for solving the Schroedinger equation (Eq. (1) or (2)) for p^--H scattering depend on the energy of the incident p^-. Described and compared in the following sections are three particular methods that are valid in different portions of the energy range from zreo to MeV energies.

3. Semiclassical Method for p^- Energy Above 10 eV

When that energy of the p^- is high, the dependence of the wave function Ψ or ψ on the position of the p^- is very strong, so a superposition of solutions in a narrow range of energies around a mean value, E, makes the p^- portion of the wave function very compact. Thus, the p^- can be represented, to a good approximation as a classical point particle. The p^- is then taken to move on a classical trajectory, and Eq. (1) is solved for the H atom only, under the time dependent influence of the p^-. Thus, for the hydrogen atom, one solves

$$-i\,\partial\Psi[\mathbf{r},t]/\partial t = (-(1/2\mu_e)\nabla_r^2 - 1/r - 1/R[t] + 1/\rho[t])\,\Psi[\mathbf{r},t] \,, \tag{6}$$

where $\rho[t] = |\mathbf{R}[t] - \mathbf{r}|$, with **R** and **r** being the vectors corresponding to R and r, and concurrently, one calculates **R**[t] (and thus R[t]) by calculating the classical trajectory of the p in a potential energy field given by

$$V[t] = -1/R + \int \Psi^*[\mathbf{r},t](1/\rho)\Psi[\mathbf{r},t]\, d\tau_r \,. \tag{7}$$

Eq. (6) and the classical trajectory are solved simultaneously by numerical methods in increments of time. Eq. (6) may be solved directly or one may use $\Psi = \Sigma_i\, c_i[t]\psi_i$, where the ψ_i are a limited set of bound and unbound states of H, and then solve for the $c_i[t]$. At

sufficiently high energies the p^- may be simply presumed to move on a straight line with a constant speed.

An example of results employing this semiclassical, time dependent approximation are shown in Fig. 1. as curves a. Experimental data on the ionization exists above 30 eV and the calculation agrees fairly well with them. These results were obtained by Schultz et al. [1] by solving Eq. (6) on a 135^3 3D cartesian spatial lattice with a constant spacing of 0.385 atomic units. Spatial differencing was accomplished by either a low order 3-point scheme or by using a high order Fourier collocation representation. Time propagation from time to t_o time t was handled by a unitary, implicit method involving expansion of the exponential time propagator, $\exp[-iH[(t+t_o)/2](t-t_o)]$. Various approximations in the numerical methods were employed. The numerical calculation was at the limit of being doable, and appears to be prohibitive for energies below 10 eV. Equation (7) was not solved directly. The p^- was assumed to move on a trajectory determined from the ground state adiabatic potential energy curve (see following section). This approximation appears to be valid at energies where the trajectory departs significantly from a straight line with the p^- moving at constant speed. This method is also valid for E> 1MeV.

Variations of the above method has been applied to other systems by a number of authors including Ritchie [2].

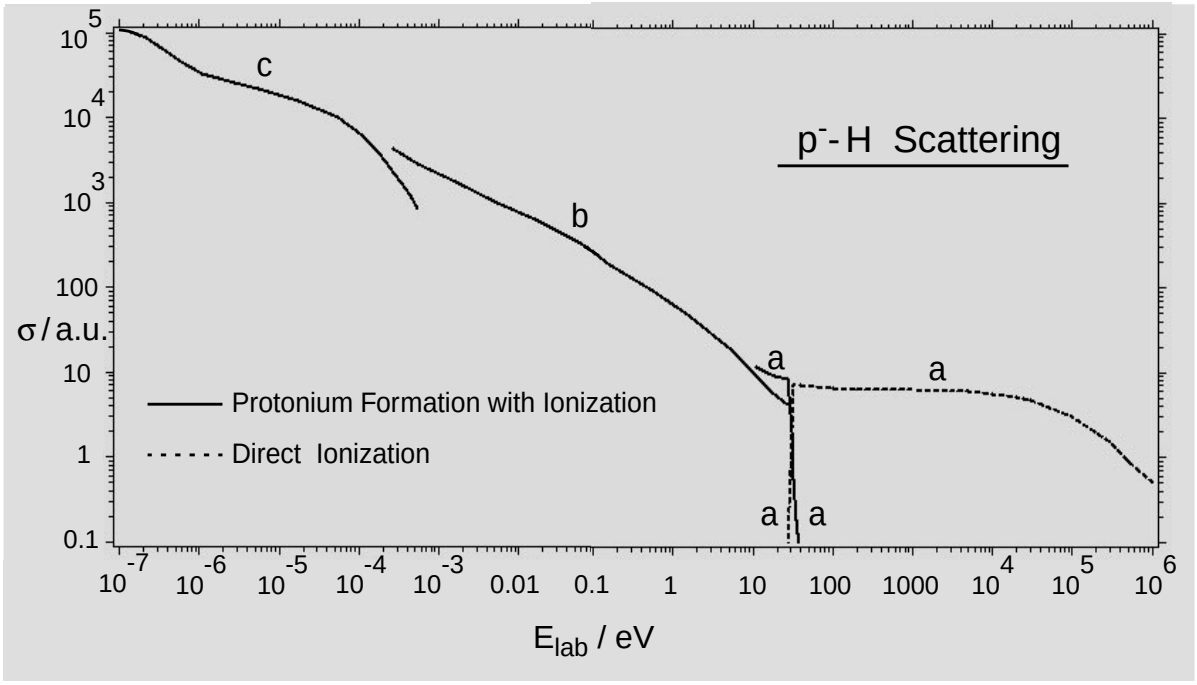

Fig. 1. Protonium formation and e^- ionization cross sections in atomic units for p^--H scattering as functions of the kinetic energy in eV in the lab frame of reference. a: Schultz et al. [1] using the semiclassical method and solving the time dependent Schroedinger equation. b: Morgan and Hughes [4] and Morgan [5] using the semiclassical method and the adiabatic approximation. c: Voronin and Carbonell [7] using a fully quantum mechanical method to solve the time independent Schroedinger equation.

4. Semiclassical Method for p^- Energy Below 10 eV

For energies around and below 10 eV another approximation is valid. That is the adiabatic approximation, which applies when the p^- is moving so slowly that the time dependent solution, Ψ, to Eq. (6) differs little (except for an insignificant multiplication factor, exp[iEt]) from the ground state solution, ψ, of the time independent equation,

$$(- (1/2\mu_e)\nabla_r^2 - 1/r - 1/R + 1/\rho\ )\ \psi[\mathbf{r}] = E\psi[\mathbf{r}]\ , \qquad (6)$$

which is just the time independent Schroedinger equation for H in the presence of a stationary p^-. Equation (6) has been considered and solved, using nearly analytic numeric means, by a number of authors including those listed in Ref. [3]. In Eq. (6), R acts as a parameter upon which ψ and E depend. The potential energy felt by the p^- is E[R] - E[∞], where E[∞] = -1/2 is the ground state energy of H (atomic units). The results of solving equation (6) may be combined with the semiclassical approximation to considerably simplify obtaining the cross section for protonium formation below 10 eV.

To employ this semiclassical, adiabatic method one proceeds as follows. First, one notes that solving Eq. (6) shows that for R less than R_c = 0.639 a.u. (atomic units) the electron becomes unbound. Thus, if the inner turning point of the p^- orbit is less than this value, the e^- leaves, and to conserve energy the p^- must become bound to the p and protonium is formed (p^- capture). Thus, one can determine the maximum value of impact parameter (R_1, distance of closest approach to the p if the p^- were moving on a straight path) which leads to the inner turning point being less than R_c. The cross section for protonium formation, σ, is then just given by

$$\sigma = \pi R_1^2. \qquad (7)$$

Morgan and Hughes [4] employed this method to determine σ and those results were later extended by Morgan [5] to somewhat higher energies. They are shown as curve b in Fig. 1. These are evidently the only results in this energy range.

Considerations concerning the accuracy and range of validity of the results are as follows. First, the adiabatic approximation breaks down as the p^- speeds up while approaching the p. This breakdown is what allows the e^- to escape and p^- to become bound, since otherwise the e^- would return and the p^- leave. There is nevertheless a probability that this reversion to the original state may occur. Morgan has made of rough estimate of this and found the probability of reversion to be nearly independent of energy below about 2 eV and about equal to 20% [6].

Second, below about 2 eV and due to the effect of the R^{-4} dependence of the long range potential energy between the p^- and H, the inner turning point is a discontinuous function of the impact parameter such that it is either well outside of R_c or well within it. Thus, around and above 2 eV, the border between protonium forming or not is less well defined, there is less time for it to occur, and calculation of the reversion probability is suspect. Thus, the results for p^- energies around and above 2 eV are probably less accurate than for those below. Further, Eq. (7) does not account for the fact that around

and above 25 eV the cross section drops rapidly to zero because the electron cannot take away the larger excess energy required for protonium formation. The upper end of validity for Eq. (7) and curve b of Fig. 1 is probably, therefore, a few to 10 eV.

The lower end of the energy range of validity is determined by the point at which assuming classical motion for the p^- becomes invalid. This lower end may be at about 10^{-4} eV where the p^- wave packet is about the same size as the H atom. However, as the p^- approaches the p, it speeds up considerably, attaining a kinetic energy well above that value, and it becomes more compact. Thus, the semiclassical, adiabatic approximation may be valid at still lower energies. It should be noted that it agrees at least roughly with the other two curves in Fig. 1 near both of its limits.

Another possible problem with this method is that it makes no account of the discrete energy states in which the protonium is formed (principal quantum numbers of about 25 to 30). A more fully quantum mechanical method for this energy range could take that into consideration. A colleague, Burke Ritchie, and I are currently searching for such a method that is capable of numerical solution with available computational methods and computers.

5. Fully Quantum Method for p^- Energy Below 10^{-4} eV

For p^- energies below 10^{-4} eV only a few p^- angular momentum waves are involved in the interaction, so it is possible to do fully quantum mechanical calculations. A. Yu. Voronin and J. Carbonell have carried out a successful, and evidently the only, such calculation.

They start by employing a unitary coupled-channel approach in which the time independent ψ is expressed as an expansion,

$$\psi[\mathbf{r},\mathbf{R}] = \phi[\mathbf{r}]\,\chi[\mathbf{R}] + \Sigma_i\, g_i[\mathbf{r}]\, f_i[\mathbf{R}]\,, \qquad (8)$$

which is to be a solution of Eq. (2) and where ϕ is the ground state wave function of H, χ is unknown, the g_i are unknown (except they are orthogonal to ϕ), and the f_i are the complete set of wave functions (eigenstates) of protonium. In Eq. (8) **r** is defined as in Section 2. above, while **R** is initially defined as the distance from the p^- to the center of mass of the p and e^-. This alternative definition leads to the absence of the gradient product in Eq. (4) and a slight change in the coefficient of ∇_R^2 there, if the **R** there is replaced by this alternative one. As it stands, there are no approximations in Eq. (8).

Voronin and Carbonell then argue that it is a good approximation to replace their initial R with the one of Section 2. while keeping the simplifying changes to the equations there that their initial choice provided. Doing so leads to simplification of the boundary conditions that were inherent in their initial choice.

Substitution of Eq. (8) into Eq. (2) and subsequent projection onto ϕ and each of the f_i then results in an infinite set of coupled 3-coordinate partial differential-integral equations which, of course, cannot be solved numerically at present. Thus they proceed through a number of approximations and substitutions to render the system tractable to

solution. First they truncate the expansion in Eq. (8) and approximate the effect of the dropped terms by adding a long range potential energy term to the equation for χ. Next they separate out the dependences of χ and the f_i on the angles of **r** and **R** (temporarily greatly multiplying the number of equations) while noting that, due in part to the low p^- energy, the f_i need only include states of low angular momentum and a limited range of principal quantum numbers. Thus, the equations are reduced to a set of coupled ordinary differential-integral equations.

That set is still numerically difficult, but the full set need only be solved once, for zero p^- energy, because a number of terms can be grouped into a complex potential energy that is nearly independent of the p^- energy. The zero-energy solution provides an evaluation of that potential energy, and when it is substituted in for other energies, the set of equations reduces to a single one which can be readily solved numerically. Considering only protonium states with angular momentum quantum numbers of one and two, their results for the protonium formation cross section are shown as curve c in Fig. 1. The adiabatic, semiclassical results agree with these very low energy results roughly around 10^{-4} eV. It is possible that inclusion of higher angular momentum states in the calculation at 10^{-4} eV might be of some significance and improve this agreement.

5. Conclusion

At the present time, the p^--H scattering problem has required a great amount of effort to render it tractable to numerical solution. This is in considerable contrast to bound state problems involving even larger numbers of particles, such as the energy states of atoms, where tractable and accurate numerical methods (variational, Hartree-Fock,....) have existed for many years.

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